NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Thermophillic Protein Stability Explained

Objective: Complete understanding of protein dynamics via simulation.

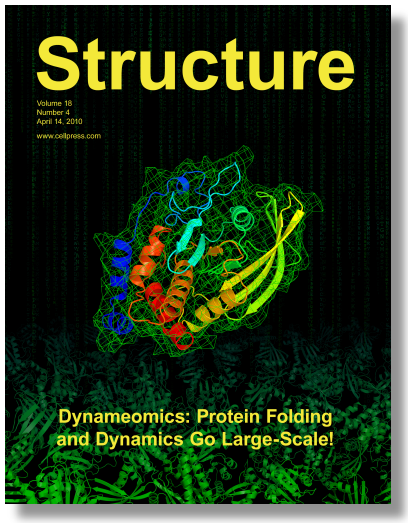
Implications: A broad knowledgebase of structural pathways to support research in bioenergy production, environmental remediation, and carbon cycling.

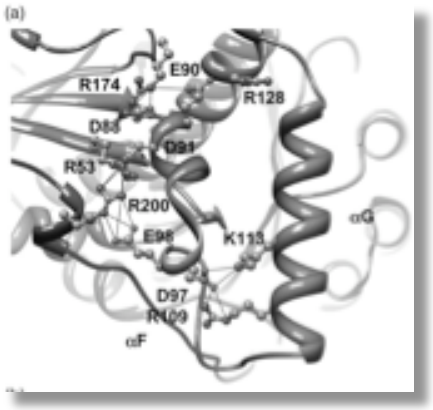
Accomplishments: Helped explain the stability of thermophilic proteins (proteins from organisms that thrive at high temperatures, up to ~176 °F).

- Simulation results for >2,000 systems stored in an innovative database linked to other sources of biological and experimental data.

NERSC: in-house simulation software, ***in lucem molecular mechanics*** (ilmm) on Franklin & Hopper

V. Daggett (U of Washington)





Left: Dynameomics journal cover story; article explained how the database can be mined to obtain insight into a variety of biologically relevant questions. Right: computed structure of a thermophilic enzyme showing why it retains its native conformation at high temperatures to a much greater degree than do other proteins.

Structure 18 (4) April 2010;
Protein Engineering Design and Selection 2010 23(5):327-336

U.S. DEPARTMENT OF ENERGY | Office of Science | BER

BERKELEY LAB